Swiss Numerical Analysis Day 2015

Université de Genève
Friday, April 17, 2015

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INVITED PLENARY SPEAKERS:
- Prof. Christian Lubich (University of Tübingen)
- Prof. Andrew Stuart (University of Warwick)

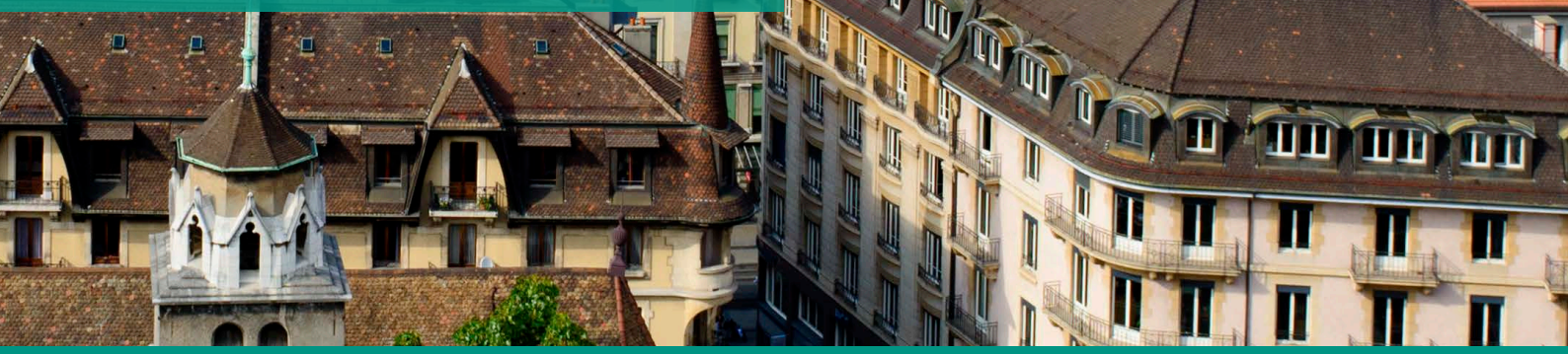
TOPICS:
Scientific computing, numerical analysis, high-performance computing, visualization, numerical analysis in engineering, computational chemistry, biology, etc.

REGISTRATION
http://colloqnum15.unige.ch
Abstract submission deadline: **March 27, 2015**
Registration deadline: **April 6, 2015**

VENUE:
Université de Genève, Uni Bastions
Lecture hall B106 (first floor)
5 rue De-Candolle, 1205 Genève, Switzerland

ORGANIZATION:
Martin Gander, Bart Vandereycken, Gilles Vilmart
(University of Geneva, Section of Mathematics)

We look forward to seeing you in Geneva!



FACULTÉ DES SCIENCES
SECTION DE MATHÉMATIQUES

UNIVERSITÉ DE GENÈVE

Swiss Numerical Analysis Day 2015
colloqnum15.unige.ch

Geneva, Switzerland
April 17, 2015

Organized by:

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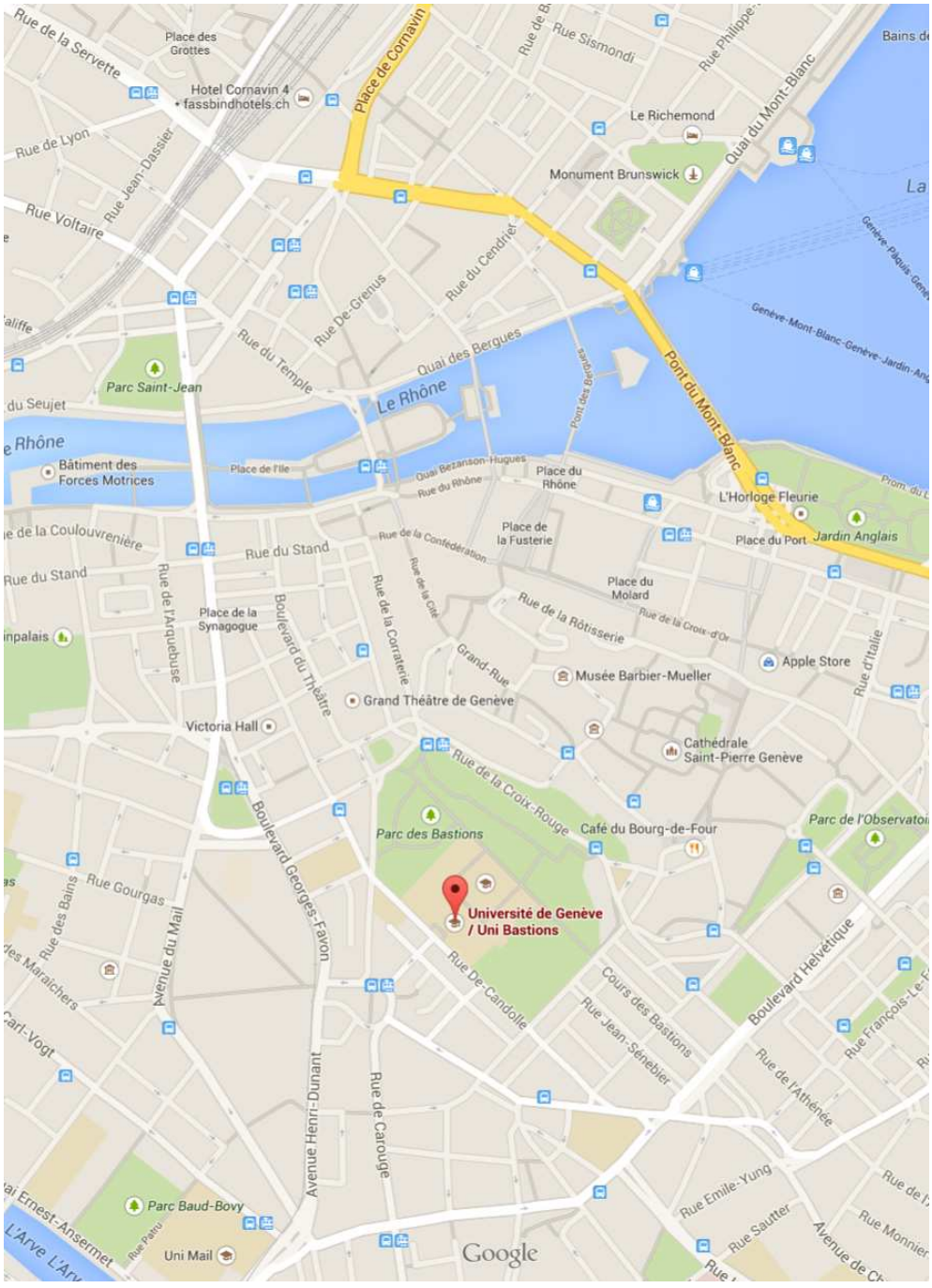
Venue: Université de Genève, Uni Bastions. Rue De-Candolle 5, 1205 Genève, Switzerland.
Uni Bastions in lecture hall B106 (first floor) on Friday 17th April 2015.

Access from the Cornavin Train Station. Take the direct tram 15 - direction Palettes, stop at Plainpalais (fourth stop). Alternatively take the direct tram 18 - direction Carouge, stop at Plainpalais (fourth stop). Both trams require a ticket “Tout Genève” (3.- swiss francs).



Swiss Numerical Analysis Day 2015 Timetable

Friday April 17th, 2015

Université de Genève, Uni Bastions. **Lecture hall B106** (first floor) Rue De-Candolle 5, 1205 Genève.

In front of **Room B106** 09:30 – 09:50	**Registration**

Room B106	
09:50 – 10:00	**Opening**
10:00 – 10:50	**Christian Lubich** (Tübingen), Dynamical low-rank approximation.

10:50 – 11:20	**Morning break** (coffee, tea, juice, croissants)

11:20 – 12:40	**Contributed pleanary talks**
11:20 – 11:40	**Monika Weymuth** (Univ. Zurich), An adaptive local basis for elliptic problems with complicated discontinuous coefficients.
11:40 – 11:00	**Mario Amrein** (Bern), Adaptive Newton methods for semi-linear problems with singular perturbations.
12:00 – 12:20	**Vladimir Kazeev** (ETH Zurich), The approximation of singular functions with quantized-tensor finite elements in two dimensions.
12:20 – 12:40	**Lorenzo Tamellini** (Lausanne), An adaptive sparse grid algorithm for elliptic PDEs with lognormal diffusion coefficient.

In front of **Room B106** 11:40 – 14:10	**Poster session and lunch buffet**

14:10 – 15:30	**Contributed pleanary talks**
14:10 – 14:30	**Marie Kray** (Basel), Wave splitting for time-dependent scattered field separation.
14:30 – 14:50	**Sebastian Krumscheid** (Lausanne), Obtaining coarse-grained models from multiscale data.
14:50 – 15:10	**Luca Dede'** (Lausanne), Efficient BDF time discretization of the Navier-Stokes equations with VMS-LES modeling in a High Performance Computing framework.
15:10 – 15:30	**Daniel Ruprecht** (Lugano), Parallel-in-time integration with PFASST.

15:30 – 16:00	**Afternoon break** (coffee, tea, juice, cakes)

16:00 – 16:50	**Andrew Stuart** (Warwick), Probabilistic numerical methods for deterministic differential equations.

16:50 – 17:00	**Closing**

Invited plenary speaker abstracts

Dynamical low-rank approximation.

Christian Lubich
University of Tübingen

This talk reviews differential equations on manifolds of matrices or tensors of low rank. They serve to approximate, in a low-rank format, large time-dependent matrices and tensors that are either given explicitly via their increments or are unknown solutions of high-dimensional differential equations, such as multi-particle time-dependent Schrödinger equations. Suitable numerical integrators are based on splitting the projector onto the tangent space of the low-rank manifold at the current approximation. In contrast to all standard integrators, these projector-splitting methods are robust with respect to the presence of small singular values in the low-rank approximation.

The talk is based on work done intermittently over the last decade with Othmar Koch, Achim Nonnenmacher, Ivan Oseledets, Bart Vandereycken, Emil Kieri and Hanna Walach.

Probabilistic numerical methods for deterministic differential equations.

Andrew Stuart
University of Warwick, Mathematics

Numerical solutions of differential equations contain inherent uncertainties due to the finite dimensional approximation of a function. In modelling scenarios where the quantification of uncertainty is a key goal it is therefore important to study the uncertainty introduced by the numerical method, in order to determine its importance relative to other uncertainties, such as those caused by noisy data or by model error. This work is concerned with a probabilistic methodology for doing so. We demonstrate an approach which gives rise to root mean square convergence rates which are consistent with the underlying deterministic method. Furthermore, we employ the method of modified equations to demonstrate enhanced rates of convergence to stochastic or random perturbations of the original deterministic problem. Ordinary differential equations and elliptic partial differential equations are used to illustrate the approach.

This is joint work with Patrick Conrad, Mark Girolami (both Warwick, Statistics), Simo Sarkka (Aalto BECS) and Konstantinos Zygalakis (Southampton, Mathematics).

Contributed plenary speaker abstracts

Adaptive Newton methods for semi-linear problems with singular perturbations.

Mario Amrein
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We will consider an adaptive procedure for the numerical solution of general, semilinear elliptic problems with possible singular pertur- bations. Our approach combines both prediction-type adaptive Newton methods and a linear adaptive finite element discretization (based on a robust a posteriori error analysis), thereby leading to a fully adaptive Newton-Galerkin scheme. Numerical experiments underline the robustness and reliability of the proposed approach for various examples.

Efficient BDF time discretization of the Navier-Stokes equations with VMS-LES modeling in a High Performance Computing framework.

Luca Dede'
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In this work, we consider the efficient time discretization of the incompressible Navier-Stokes equations with Variational Multiscale-LES (VMS-LES) modeling of turbulence. Specifically, we spatially approximate the problem by means of the Finite Element method and use the Backward Differentiation Formulas (BDF) for the time discretization, which lead to an efficient semi-implicit treatment of the nonlinear terms of the Navier-Stokes equations with VMS-LES modeling. In this manner, the full discrete problem involves the solution of a single linear system at each time step, which we numerically solve by means of the GMRES method with a multigrid preconditioner for the High Performance Computing framework. We solve benchmark problems at high Reynolds numbers and turbulent regimes, for which we discuss the scalability results and computational efficiency of the solver in the parallel setting.

The approximation of singular functions with quantized-tensor finite elements in two dimensions.

Vladimir Kazeev
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We consider a countably-normed space of analytic bivariate functions with corner singularities. The class includes, in particular, the solutions of linear second-order elliptic problems in polygonal domains. For the functions from that class, we analyze a first-order, h-version finite-element approximation, which is well-known to converge algebraically with rate at most 1 with respect to the discretization parameter h. We prove that such functions, when the coefficient vectors are represented in the so-called quantized tensor train format, admit approximations converging exponentially with respect to the number of QTT parameters, which becomes the effective number of degrees of freedom. This allows to achieve accuracy $\varepsilon > 0$ in the energy norm of the elliptic problem with $\mathcal{O}(\log^{\kappa} \varepsilon^{-1})$ parameters in the corresponding tensor representation. We demonstrate numerically that the same holds for the FE solution resulting from the entire process of solving the Galerkin first-order FE discretization using a tensor-structured solver of linear systems.

Wave splitting for time-dependent scattered field separation.

Marie Kray
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Starting from classical absorbing boundary conditions, we propose a method for the separation of time-dependent scattered wave fields due to multiple sources or obstacles. In contrast to previous techniques, our method is local in space and time, deterministic, and also avoids a priori assumptions on the frequency spectrum of the signal.

Obtaining coarse-grained models from multiscale data.

Sebastian Krumscheid
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Many natural phenomena and technological applications are modelled by deterministic or random dynamical systems. Often, these dynamical systems are characterized by the presence of processes occurring across different length and/or time scales. Examples range from biological systems and problems in atmosphere and ocean sciences to molecular dynamics, materials science, and fluid and solid mechanics, to name but a few. Of main interest for these systems is typically only the dynamics at the longest scale and multiscale methods (e.g. averaging and homogenization) provide an analytic framework for the rigorous derivation of coarse-grained dynamical systems that represent the full multiscale systems at this scale. These analytic techniques are, however, often not applicable in practice due to the complex structure of the underlying multiscale system or simply because the multiscale system is not known entirely. Instead it is desirable to infer stochastic coarse-grained models from observational data of the underlying multiscale process. It is known that estimators such as the maximum likelihood estimator or the quadratic variation of the path estimator can be strongly biased in this setting. In this talk we discuss a novel parametric inference methodology for stochastic coarse-grained models that does not suffer from this drawback. Moreover, we exemplify through a real-world data set how these data-driven coarse-graining techniques can be used to study the statistical properties of a given temporal process.

Parallel-in-time integration with PFASST.

Daniel Ruprecht
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The explosion of core counts in modern supercomputers brings with it a multitude of very different challenges. One major issue is the demand for novel parallel numerical algorithms that can efficiently exploit the massive computing power at hand. Over the recent years, parallel-in-time integration methods have emerged as a promising approach to provide additional concurrency, extend strong scaling limits and to escape the “trap weak of scaling”. The talk will sketch the “parallel approximation scheme in space and time” (PFASST), introduced in 2012 by Emmett and Minion. It will present performance results on close to half a million cores and sketch recent algorithmic variations, interweaving PFASST with spatial multi-grid solvers to further improve performance.

An adaptive sparse grid algorithm for elliptic PDEs with lognormal diffusion coefficient.

Lorenzo Tamellini
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Solutions of PDEs depending on random parameters can be conveniently approximated by polynomial expansions over the parameter space. However, these approximations suffer from a performance degradation as the number of random parameters increases ("curse of dimensionality" effect). To minimize this effect, in this talk we consider an adaptive sparse grids algorithm and apply it to a classic benchmark test in Uncertainty Quantificaiton, i.e. the Darcy equation with random lognormal permeability field. Moreover, to treat the case of rough permeability fields, in which a sparse grid approach may not be suitable, we propose to use the adaptive sparse grid quadrature as a control variate in a Monte Carlo simulation. Numerical results will validate the proposed approach

An Adaptive Local Basis for Elliptic Problems with Complicated Discontinuous Coefficients.

Stefan A. Sauter, Monika Weymuth
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We will present a generalized finite element method for the discretization of elliptic partial differential equations in heterogenous media. In [1] a method has been introduced to set up an *adaptive local* finite element basis (AL basis) on a coarse mesh with mesh size H which, typically, does not resolve the matrix of the media while the textbook finite element convergence rates are preserved. This method requires $O(\log(1/H)^{d+1})$ basis functions per mesh point where d denotes the spatial dimension of the computational domain. Since the continuous differential operator is involved in the construction, the method presented in [1] is only semidiscrete.
We will present a fully discrete version of the method, where the AL basis is constructed by solving finite dimensional localized problems. A key tool for the discretization of the differential operator is the theory developed in [2, 3]. We will prove that the optimal convergence rates are preserved and give some complexity estimates.

References

[1] L. Grasedyck, I. Greff, and S. Sauter. *The AL Basis for the Solution of Elliptic Problems in Heterogeneous Media*. SIAM J. Multiscale Model. Simul., 10(1), 245-258, 2012.

[2] D. Peterseim and S. Sauter. *Finite elements for elliptic problems with highly varying, nonperiodic diffusion matrix*. Multiscale Model. Simul., 10(3), 665-695, 2012

[3] M. Weymuth. *Fully Discrete Version of the AL Basis for Elliptic Problems with General L^∞-Coefficient*. Institut für Mathematik, Universität Zürich, 2013, Technical Report
https://www.math.uzh.ch/compmath/index.php?id=reports.

Poster abstracts

A reduced basis multiscale method for Stokes flow in porous media.

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We present a numerical multiscale method for Stokes flow in porous media [3] that is based on homogenization [4, 5]. The method proposed in [1] applies a finite element method for solving an effective Darcy problem with permeability recovered from microscopic Stokes problems. The computational cost of this method is dominated by the repeated computation of micro problems. To address this issue, we proposed a reduced basis (RB) method for the Stokes flow on the micro scale [2, 3]. In the offline stage we use a greedy algorithm to choose a small set of representative micro solutions, the RB. Micro problems are then approximated by a Petrov-Galerkin projection to a low-dimensional solution space spanned by the RB and a parameter-dependent test space. The online stage provides a fast and stable evaluation of the output of interest (effective permeability) for any parameter value (macroscopic coordinate). Two and three dimensional numerical experiments confirm the accuracy and time cost reduction of the multiscale method.

References

[1] A. Abdulle and O. Budáč, *An adaptive finite element heterogeneous multiscale method for the Stokes problem in porous media*, Multiscale Model. Simul., (13) 2015, pp. 256–290.

[2] A. Abdulle and O. Budáč, *A Petrov-Galerkin reduced basis approximation of the stokes equation in parametrized geometries*. submitted to C. R. Math. Acad. Sci. Paris.

[3] A. Abdulle and O. Budáč, *A reduced basis finite element heterogeneous multiscale method for Stokes flow in porous media*. in preparation.

[4] G. Allaire, *Homogenization of the Stokes flow in a connected porous medium*, Asymptot. Anal., 2 (1989), pp. 203–222.

[5] E. Sánchez-Palencia, *Non-homogeneous media and vibration theory*, vol. 127 of Lecture Notes in Phys., Springer, 1980.

Comparison of Neuman-Neuman and Optimal Schwarz Methods with Many Subdomains in one Spatial Dimensions.

Faycal Chaouqui
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Optimal Schwarz methods and Neuman-Neuman methods have for two subdomains both the interesting property that they can lead to nil-potent iteration matrices. We study in this poster if this property can also be obtained for the case of a strip decomposition into many subdomains. We show that only the optimal Schwarz method can lead in this case to a nil-potent iteration matrix, and that there are various choices in the transmission conditions that lead to nil-potent matrices of different degrees.

Anisotropic error estimates and adaptive algorithm for the Crank-Nicolson method applied to an hyperbolic problem.

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A fully discrete approximation of the transport equation is studied. Stabilized continuous finite elements for space discretization and Crank-Nicolson scheme for time discretization are considered. Fully discrete a priori and a posteriori error estimates are derived in the framework of anisotropic meshes, where a quadratic reconstruction of the numerical solution is used to obtain optimal order of the error estimator in the time variable. Numerical results are presented on nonadapted meshes with small constant time steps. Sharpness of space and time error estimates are confirmed. Then space and time adaptivity is considered and an adaptive algorithm is proposed. Numerical experiments with adapted meshes and adapted time steps are performed in order to verify effectiveness and accuracy of the adaptive algorithm.

Numerical scheme for the temperature dependent dissolution of alumina in an aluminium electrolysis cell.

Thomas Foetisch
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The electrolysis cell must be fed with alumina powder to replace the alumina which is consumed by the reaction. A precise control of the local alumina concentration in the electrolyte is crucial to ensure the efficiency of the process. The dynamic of the dissolution of the powder is affected by the local alumina concentration, and by the local temperature. A numerical model is proposed to take into account the temperature dependency on the dissolution, and investigate the effect of the bath's temperature on the solved alumina concentration over the electrolyte. The temperature of the electrolyte being close to the temperature of the liquidus, taking the bath's temperature into account has an important impact on the predictions of the model.

Higher-order quasi Monte Carlo for Bayesian inverse problems.

Robert Gantner
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We consider a deterministic approach to approximating solutions to Bayesian inverse problems for the diffusion equation based on infinite-parametric representations of the diffusion coefficient. The approximation of the involved high-dimensional integrals is achieved by a higher-order quasi-Monte Carlo method achieving a rate of convergence of the error larger than 1 in the number of evaluations of the forward model. Numerical results show significant gains when comparing to a standard Monte Carlo sampling approach.

A posteriori error estimation for partial differential equations with small uncertainties.

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We present a priori and a posteriori error estimation for partial differential equations (PDEs) affected by uncertain input data characterized by random variables, or more generally by random fields. We focus on PDEs with small uncertainties and adopt a perturbation approach expanding the exact (random) solution up to a certain order with respect to a parameter that controls the amount of randomness. Uncoupled deterministic problems can be derived to find each term in the expansion, each of which can be solved approximately using for instance finite elements. We derive a priori and a posteriori error estimates for the error between the exact solution and an approximation of a certain order in various norms. For instance for the first order ap- proximation, which requires the resolution of only one deterministic problem, we derive an a posteriori error estimator constituted of two computable parts, namely a part due to finite element approximation and another part due to uncertainty. This estimator can then be used for mesh adaptation to balance the two sources of error. We first present the error analysis performed on a linear diffusion model problem with random diffusion coefficient and illustrate the theoretical results with several numerical examples. We extend then the analysis to a class of nonlinear problems and perform a comparison with the Stochastic Collocation method in terms of computational costs.

A new approach for preconditioning discontinuous Galerkin discretizations.

Soheil Hajian
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Domain decomposition preconditioners and in particular the additive Schwarz method are favorite preconditioners for classical finite element methods (FEM). There is a huge effort in designing similar preconditioners for discontinuous Galerkin (DG) discretizations. It has been shown that additive Schwarz methods use different mechanism for convergence when applied to a DG discretization compared to the classical FEM. More precisely, additive Schwarz methods, when applied to DG, use a non-overlapping Robin transmission condition for the communication between subdomains. This is exactly the same transmission condition that optimized Schwarz methods (OSM) use to obtain fast convergence. In this poster we present an OSM preconditioner for a particular DG discretization along with theoretical convergence estimates.

Numerical homogenization methods for nonlinear monotone parabolic multiscale PDEs.

Martin Huber
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We present two numerical homogenization methods for nonlinear monotone parabolic multiscale problems with data rapidly oscillating in space. First, we introduce the method from [1] combining the implicit Euler method in time with a finite element heterogeneous multiscale method in space (coupling macro and micro finite element methods). This upscaling procedure however relies on nonlinear elliptic micro sampling problems which can be computationally costly in practical applications. Second, we define a linearized scheme introduced in [2] that is much more efficient as it only involves linear micro problems. We present the fully discrete a priori error estimates derived in [1, 2] and compare the performance of the two methods.

Joint work with Assyr Abdulle and Gilles Vilmart.

References

[1] A. Abdulle and M. E. Huber, *Finite element heterogeneous multiscale method for nonlinear monotone parabolic homogenization problems*. MATHICSE Technical Report 31.2014, École Polytechnique Fédérale de Lausanne.

[2] A. Abdulle, M. E. Huber, and G. Vilmart, *Linearized numerical homogenization method for nonlinear monotone parabolic multiscale problems*. To appear in Multiscale Model. Simul.

Schur complement approximation via multi-grid methods.

Lukas Jakabcin
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We propose an approximation of the Schur complement for an elliptic problem using multi-grid prolongation and restriction operators. In particular, we define an approximate Schur complement operator and study the approximation numerically. We also present an operator estimate for a 2-grid approximation.

An optimization-based coupling method for multiscale problems.

Orane Jecker
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An optimization based method is proposed for solving multiscale problems, with non scale separation in some region of the computational domain. The method couples a fine scale solver, in the subregions without scale separation, with a micro-macro method, in regions where an effective solution can be computed. Introducing an overlap region, the method is written as a minimization problem constrained by boundary value problems in each subregion, with virtual controls (unknown Dirichlet data) as boundary data in the overlap. The virtual control are obtained by minimizing the L2 norm of the difference between the solutions in the overlap. A priori error estimates are discussed and a numerical experiment, illustrating the theoretical convergence rate, is presented.

Octree-based adaptive solver for the transport equation.

Viljami Laurmaa
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A numerical scheme for solving the transport equation using an adaptive octree structure is presented. A VOF-type approach is used to track the fluid and the octree is refined at the interface for accurate tracking. Advection is done using a semi-Lagrangian scheme where we translate the cells along the characteristics and project them back on the octree. This approach does not require the usual CFL condition for stability and allows large timesteps. Consequently, the scheme is computationally fast and the adaptivity allows low memory usage.

Approximation of admissible measure valued solutions for incompressible Euler equations.

Filippo Leonardi
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We propose a new numerical scheme for the solution of incompressible Euler equations. This scheme has a number of interesting properties, which mimic the behaviour of the governing equations. We also propose a procedure, which allows a consistent approximation of admissible measure valued solutions.

Optimized Schwarz methods for second order and biharmonic elliptic problems.

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We study a two sided Optimized Schwarz method with an additional relaxation step for a second order elliptic problem. Our analysis for a two subdomain decomposition shows that the optimal choice of the Robin parameters is $p_1 = 0$ and $p_2 = +\infty$, or $p_1 = +\infty$ and $p_2 = 0$, which results in the Dirichlet-Neumann method. Fixing however one parameter p_i, $i = 1, 2$, we find that the optimal choice of the other parameter minimizing the contraction factor satisfies $p_1 p_2 = \text{const}$.

We next study an Optimized Schwarz method for the biharmonic equation. Through a suitable choice of the parameters, we obtain that the optimal convergence rate is exactly the same as for the second order elliptic problem, and is much better than for the classical Schwarz method.

Low-rank tensor methods for communicating Markov processes.

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A number of practical applications lead to Markov Chains with extremely large state spaces. Such an instance arises from models for calcium channels, which are structures in the body that allow cells to transmit electrical charges to each other. These charges are carried on a calcium ion which can travel freely back and forth through the 'calcium channel'. The state space of a Markov process describing these interactions typically grows exponentially with the number of cells. More generally, Stochastic Automata Networks (SANs) are networks of interacting stochastic automata. The dimension of the resulting state space grows exponentially with the number of involved automata. Several techniques have been established to arrive at a formulation such that the transition matrix has Kronecker product structure. This allows, for example, for efficient matrix-vector multiplications. However, the number of possible automata is still severely limited by the need of representing a single vector (e.g., the stationary vector) explicitly. We propose the use of low-rank tensor techniques to avoid this barrier. More specifically, some algorithms are presented that allow to approximate the solution of certain SANs very efficiently in a low-rank tensor format.

Hierarchical matrices, or H-matrices.

Parisa Mamooler
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Numerical analysts avoid whenever possible to work with large dense matrices. Instead, they try to approximate them with sparse or low rank matrices. H-matrices are one of these methods which use data-sparse approximations of non-sparse matrices. In fact, they provide tools to perform matrix operations in almost linear complexity (of $O(nk \log n)$). One of the important properties of the H-matrices is that they are valid for the important class of matrices originating from standard discretisations of elliptic partial differential equations or the related integral equations. We show in this poster the basic ideas of H-matrices and their application for solving an integral equation, and also explain continuous versions of matrices, called quasi-matrix and cmatrix, and their LU factorisation, in view of formulating continuous H-matrices.

Runge-Kutta type Explicit Local Time-Stepping Methods for Electromagnetics.

Michaela Mehlin
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The efficient and accurate numerical simulation of time-dependent Maxwell's equations is of fundamental importance in electromagnetic wave propagation. Following the method-of-lines approach we first discretize Maxwell's equations in space using nodal discontinuous Galerkin (DG) finite element methods (FEM). FEM are increasingly popular in the presence of heterogeneous media or complex geometry due to their inherent flexibility: elements can be small precisely where small features are located, and larger elsewhere. Such a local mesh refinement, however, also imposes severe stability constraints on explicit time integration, as the maximal time-step is dictated by the smallest elements in the mesh. When mesh refinement is restricted to a small region, the use of implicit methods, or a very small time-step in the entire computational domain, are generally too high a price to pay. Starting from explicit Runge-Kutta(RK) methods, we propose high order explicit local time-stepping (LTS) methods for the simulation of electromagnetic wave phenomena. By using smaller time steps precisely where smaller elements in the mesh are located, these LTS methods overcome the bottleneck in explicit time integration caused by local mesh refinement, without sacrificing the explicitness, accuracy or efficiency of the original RK method.

Discrete Duality Finite Volume (DDFV) method applied to COSMO horizontal diffusion.

Sandie Moody
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At present, the horizontal components of the subrid scale flux divergence of the averaged equation for mass of water constituents are not being calculated in the COSMO-Model. This is due to the calculation method, whose stability is limited. We propose a new calculation method, a coupling of the DDFV and finite volume methods, to be implemented in the COSMO-Model. Our results show that the DDFV method is adapted to the COSMO-Model as it is stable on any grid type, in particular a terrain-following grid including steep slopes. We also analyse computational costs and convergence rates.

Finite Elements for Wave Propagation in polygonal domains.

Fabian Müller
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When dealing with propagation phenomena of acoustic or seismic waves, second-order linear wave equations provide a commonly used physical model. The method of lines is a popular simulation technique. There, the partial differential equation (PDE) is discretized in space first, followed by a time-stepping scheme solving the resulting ordinary differential equation. When using a Finite Element method (FEM) for the spatial discretization, the convergence order strongly depends on the regularity of the solution. When dealing with a PDE posed on a polygonal domain or in the presence of piecewise smooth coefficients ('wavespeeds'), the solution exhibits strongly singular behaviour in the neighbourhood of an isolated point set, implying slow convergence of the FEM on quasi-uniform meshes. Recently, we have proved that quasi-optimal convergence rates can be obtained again for the h-version of FEM with arbitrarily high local

polynomial degree. We present results which are applicable to acoustic and elastic wave equations in homogeneous media, as well as the acoustic wave equation in a heterogeneous medium, i.e. in the presence of piecewise smooth wavespeeds.

Adaptive Eigenspace Inversion for the Helmholtz Equation.

Uri Nahum
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An adaptive inversion method was presented in [M. de Buhan,M. Kray, inverse problems, 2013] for time-dependent inverse scattering problems set in a (known)constant background medium. Here we extend that approach to a general varying background in the frequency domain, while dispensing with the need for an open observational subset. The resulting adaptive eigenspace inversion (AEI) method not only proves more accurate and robust to missing data, but also incurs only a fraction of the computational cost.

Shape optimization of micro lenses.

Alberto Paganini
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Micro lenses are optical structures exhibiting interesting effects caused by internal resonances. These effects cannot be computed with geometric optics because micro lenses are not much larger than the wavelength of the incident light. For this reason, optimizing their design is a challenging task. We apply a shape optimization algorithm tailored for finite element simulations to improve the optical properties of an initial design. The algorithm enjoys superconvergent domain integral expressions for the shape gradient, and allows for arbitrarily high resolution of shapes by employing B-spline based representations of the deformation diffeomorphism.

Auxiliary Space Preconditioners for H(curl)-elliptic Problems with Discontinuous Coefficients.

Blanca Ayuso de Dios[1], Ralf Hiptmair[2], Cecilia Pagliantini[3] [1] Dipartimento di Matematica, Università di Bologna, Italy
[2] Seminar for Applied Mathematics, ETH Zürich, Switzerland
[3] Seminar for Applied Mathematics, ETH Zürich, Switzerland
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We propose a family of preconditioners to solve the linear systems of equations ensuing from a symmetric Interior Penalty Discontinuous Galerkin (DG) discretization of H(curl)-elliptic boundary value problems arising in eddy current models. The design and analysis of the proposed solvers relies on the auxiliary space method: The preconditioners are obtained for the non-conforming DG approximation by using an auxiliary space of H(curl)-conforming finite elements together with a relaxation technique (smoother).

Specifically, we address the influence of possible discontinuities in the diffusivity ν and/or in the reaction coefficient β on the asymptotic performance of the preconditioners. Asymptotic optimality and robustness with respect to jumps in the coefficients and the mesh size can be shown, except when both coefficients are discontinuous and the problem is curl-dominated in some regions and reaction dominated in others. In this

latter case the convergence depends on the minimum among the ratio $h^2\beta/\nu$, the jumps in β and the jumps in ν.

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Parallel solver for the space in homogeneous and time dependent Boltzmann equation.

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We present a high-performance implementation for the solution of the space in homogeneous and time dependent Boltzmann equation. The phase space is discretized using finite elements for the physical domain and a polar spectral discretization based on Laguerre polynomials in velocity. Computations are done 2+2+1 dimensions with an implicit/explicit split time stepping scheme on unstructured meshes. The polar spectral scheme can be made fully conservative and requires no truncation of the collision operator.

Numerical Approximation of Turbulent Flows in Electrolysis Cells.

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Aluminium is a metal extracted from bauxite ore using electrolysis process, called Hall-Héroult process, and is done in a electrolytic bath within a huge cell. Observations and measurements are difficult to make in the cell and in this context numerical simulation can be very useful to optimize the production. The modeling of the electrolysis process is a two fluids system (liquid aluminium and electrolytic bath) with free moving interface. In this work we focus on the magnetohydrodynamic (MHD) computation of the motion of the fluid and interface. Mixing length turbulent models and projection methods to solve the Navier-Stokes equations are presented.

Shape uncertainty quantification for scattering transmission problems.

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We consider the *Helmholtz transmission problem* with an incoming plane wave, where the shape of the scatterer is affected by random perturbations; the latter are the only source of uncertainty in our model problem.

Since we are interested in shape fluctuations that are too large for being treated via a perturbative method, we use instead a probabilistic description of the interface to parametrize it through a *deterministic, high-dimensional parameter* incorporating the shape randomness.

Using a domain mapping approach, we introduce a parameter-dependent map to refer each domain realization to a *nominal* configuration, fixed for all realizations. In this way, we can write a variational formulation on the nominal configuration with parameter-dependent coefficients, a framework for which theory and discretization algorithms are well established.

For the discretization in the parameter space, we present an adaptive Smolyak algorithm for sparse stochastic collocation [1], which allows to achieve quasi-optimal convergence rates (with respect to the

best N-term approximation) and does not suffer from the so-called 'curse of dimensionality'. We show that the solution on the nominal space and linear functionals of it satisfying certain hypothesis fulfill the assumptions required by the convergence theorems, in particular as regards the analytic dependence on the high-dimensional parameter. The spatial discretization at each collocation point is performed using Finite Elements.

In the numerical experiments, we consider two settings: a particle in free space and a particle on substrate. When addressing the interpolation and quadrature of the real part the solution in the *nominal* space and of the far field functional, the theoretical convergence rates are achieved.

However, if we address the quadrature on the *physical* domain, then, due to the presence of the interface, the analytic dependence of the solution on the high-dimensional parameter breaks down; in such a case, the sparse adaptive Smolyak algorithm does not converge anymore and alternative techniques are required. We show this on a couple of simple examples.

This work is part of a PhD thesis under the supervision of Prof. Ralf Hiptmair and Prof. Christoph Schwab, and with the collaboration of Dr. Claudia Schillings.

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A Reduced Basis approach to large-scale pseudospectra computation.

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When studying spectral properties of a non-normal matrix $A \in \mathbb{C}^{n\times n}$ information about its spectrum alone is usually not enough to provide complete information. Effects of small perturbations on $\sigma(A)$ can be studied by computing so-called ϵ-pseudospectra. For $\epsilon > 0$ the ϵ-pseudospectrum of A is usually defined as

$$\sigma_\epsilon(A) = \{z \in \mathbb{C} : \|(zI - A)^{-1}\|_2 > \epsilon^{-1}\},$$

or

$$\sigma_\epsilon(A) = \{z \in \mathbb{C} : \sigma_{\min}(zI - A) < \epsilon\}.$$

The computation of $\sigma_\epsilon(A)$ requires the evaluation of the function $g(z) = \sigma_{\min}(zI - A)$ on a portion of the complex plane. For $z = x+iy$, the computation of $g(z)$ can be seen as a 2-dimensional parameter-dependent eigenvalue problem:

$$g(x + iy)^2 = \lambda_{\min}\left(((x + yi)I - A)^*((x + yi)I - A)\right).$$

In this work, we propose a Reduced Basis approach to pseudospectra computation that provides highly accurate estimates of pseudospectra in the region of interest. It incorporates the sampled singular vectors of $zI - A$ and implicitly exploits their smoothness properties. It provides rigorous bounds, both upper and lower, on the pseudospectra in the region of interest.

Second-kind Boundary Element Methods for Scattering at Partly Impenetrable Objects.

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We present a second-kind Galerkin formulation for transmission problems in acoustic scattering at partly impenetrable composite objects. The bounded composite scatterer consists of several Lipschitz polyhedra characterizing the homogeneous materials. Impenetrable parts are introduced by imposing Dirichlet boundary conditions on the boundary of some of the Lipschitz polyhedra.

The popular PMCHWT formulation, a first-kind boundary element method proposed in [3], leads to ill-conditioned linear systems on fine meshes, with no effective preconditioner available yet.

Our second-kind approach provides an alternative that is intrinsically well-conditioned. We represent the total field through a global multi-potential consisting of the sum of all local potentials from the homogeneous parts of the scatterer. This ansatz leads to a second-kind boundary integral equation in L^2 for the Cauchy trace of the total field at the material interfaces. Ritz-Galerkin discretization with any kind of L^2-stable trial and test functions yields well-conditioned linear systems which can be solved efficiently with iterative solvers.

Numerical tests with piecewise constant boundary elements confirm the good conditioning of the Galerkin matrices of our approach and therefore fast convergence of iterative solvers like GMRES. Via L^2-projection of the computed Dirichlet trace onto continuous piecewise linear boundary elements, we achieve competitive accuracy when comparing with the popular first-kind formulation.

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Riemannian Optimization for High-Dimensional Problems.

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The development of efficient numerical methods for high-dimensional problems is a highly active area of research in numerical analysis and numerical linear algebra. High dimensionality occurs in several scientific disciplines and may have a variety of causes. In this presentation, we focus on two problems that appear when dealing with such problems. In the first part, tensor completion, we aim to reconstruct a high-dimensional data set with a large fraction of missing entries. In the second part, we focus on the solution of very large linear systems, a challenging task often encountered as a core ingredient when solving partial differential equations on high-dimensional domains. In these cases, the degrees of freedom grow exponentially with the number of dimensions, making classic approaches unfeasible. Approximation of the

solution by low-rank tensor formats often allows us to avoid this curse of dimensionality by exploiting the underlying structure. The assumption of low-rank structure in the model allows us to cast these problems into optimization problems restricted to the manifold of fixed-rank tensors. Elements of this smooth embedded submanifold can be efficiently represented in the Tucker or tensor train (TT) formats, with storage complexity scaling linearly with the number of dimensions. For tensor completion, we present a nonlinear conjugate gradient scheme within the framework of Riemannian optimization which exploits this favorable scaling. Numerical experiments and comparison to existing methods show the effectiveness of our approach for the approximation of multivariate functions. Furthermore, we show that our algorithm can obtain competitive reconstructions from uniform random sampling of few entries of compared to adaptive sampling techniques such as cross-approximation. For linear systems, we propose a new algorithm that performs a preconditioned gradient method on the manifold of tensors of fixed rank. We demonstrate the flexibility of our algorithm by comparing different approximations of the Riemannian Hessian as preconditioners for the gradient directions.

On low rank updates of matrix functions.

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The efficient and reliable update computation of large-scale matrix functions subject to low-rank perturbations is of interest in several applications, such as the analysis of networks. For addressing this problem, Beckermann and Kressner have proposed the use of tensor polynomial and rational Krylov subspace methods. Starting from the exactness property of (rational) Krylov subspaces, convergence bounds for the tensor Krylov subspace method have been derived. In particular, we discuss $\exp(A)$ and $\mathrm{sign}(A)$. The matrix sign function immediately yields the corresponding spectral projector, which can be used in the solution of eigenvalue problems. For the case of the matrix exponential, the error expansion in terms of $\varphi-$ functions as well as the resulting corrected scheme proposed by Saad are extended to the tensor Krylov subspace method. While the corrected scheme itself may not offer advantages, it has been observed useful in deriving stopping criteria.

Optimized Schwarz Methods for Heterogeneous Harmonic Waves.

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We perform Schwarz Algorithms to solve Maxwell's and Helmholtz equations in heterogeneous media, we consider the discontinuity of the coefficients aligned with the interface between subdomains. We show that the jump in the coefficients helps to the convergence of the algorithm if it is taken in account carefully, in most of the cases it makes the convergence independent of the mesh size of the discretisation. We show numerical examples to verify the results.

Factorizations, Sweeping, Source Transfer, Potentials and Schwarz: One Algorithm.

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It is not surprising that one algorithm can be devised by different means and be stated in apparently different formulations but actually do the same thing. This is especially interesting for the recent emerging algorithms for the iterative solution of the Helmholtz equation such as the sweeping preconditioners, the source transfer and the single and/or double layer potential based methods. We will see how these algorithms resemble and differ in terms of optimized Schwarz methods.

co-authored with Martin J. Gander.

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- Remi Abgrall (University of Zurich)
- Mario Amrein (University of Bern), **Contributed plenary speaker** (see p.9)
- Maboudi Afkham Babak (EPF Lausanne)
- Paola Bacigaluppi (University of Zurich)
- Adrian Blumenthal (EPF Lausanne)
- Jean-Paul Berrut (University of Fribourg)
- Julien Bodelet (University of Geneva)
- Charles-Edouard Brehier (University of Neuchatel)
- Ondrej Budac (EPF Lausanne), **Poster** (see p.13)
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- Sandie Moody (University of Geneva), **Poster** (see p.18)
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